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LIFE CYCLE MANAGEMENT

Enabling optimization in LCA: from "ad hoc" to "structural" LCA approach—based on a biodiesel well-to-wheel case study

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Abstract
Purpose Applied life cycle assessment (LCA) studies often lead to a comparison of rather few alternatives; we call this the "ad hoc LCA approach." This can seem surprising since applied LCAs normally cover countless options for variations and derived potentials for improvements in a product life cycle. In this paper, we will suggest an alternative approach to the ad hoc approach, which more systematically addresses the many possible variations to identify the most promising. We call it the "structural LCA approach." The goals of this paper are (1) to provide basic guidelines for the structural approach, including an easy expansion of the LCA space; (2) to show that the structural LCA approach can be used for different types of optimization in LCA; and (3) to improve the transparency of the LCA work.
Methods The structural approach is based on the methodology "design of experiments" (Montgomery 2005). Through a biodiesel well-to-wheel study, we demonstrate a generic approach of applying explanatory variables and corresponding impact categories within the LCA methodology. Explanatory variables are product system variables that can influence the environmental impacts from the system. Furthermore, using the structural approach enables two different possibilities for optimization: (1) single-objective optimization (SO) based on response surface methodology (Montgomery 2005) and (2) multiobjective optimization (MO) by the hypervolume estimation taboo search (HETS) method. HETS enables MO for more than two or three objectives.
Results and discussion Using SO, the explanatory variable "use of residual straw from fields" is, by far, the explanatory variable that can contribute with the highest decrease of climate change potential. For the respiratory inorganics impact category, the most influencing explanatory variable is found to be the use of different alcohol types (bioethanol or petrochemical methanol) in biodiesel production. Using MO, we found the Pareto front based on 5 different life cycle pathways which are nondominated solutions out of 66 different analyzed solutions. Given that there is a fixed amount of resources available for the LCA practitioner, it becomes a prioritizing problem whether to apply the structural LCA approach or not. If the decision maker only has power to change a single explanatory variable, it might not be beneficial to apply the structural LCA approach. However, if the decision maker (such as decision makers at the societal level) has power to change more explanatory variables, then the structural LCA approach seems beneficial for quantifying and comparing the potentials for environmental improvement between the different explanatory variables in an LCA system and identifying the overall most promising product system configurations among the chosen PWs.

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Conclusions The implementation of the structural LCA approach and the derived use of SO and MO have been successfully achieved and demonstrated in the present paper. In addition, it is demonstrated that the structural LCA approach can lead to more transparent LCAs since the potentially most important explanatory variables which are used to model the LCAs are explicitly presented through the structural LCA approach. The suggested structural approach is a new approach to LCA and it seems to be a promising approach for searching or screening product systems for environmental optimization potentials. In the presented case, the design has been a rather simple full factorial design. More complicated problems or designs, such as fractional designs, nested designs, split plot designs, and/or unbalanced data, in the context of LCA could be investigated further using the structural approach.

Keywords Design of experiments · LCA · Optimization · Rapeseed biodiesel · Structural approach

1 Introduction

Life cycle assessment (LCA) offers a quantitative approach to assess environmental impacts from products, technologies, and services (Wenzel et al. 1997; Finnveden et al. 2009; European Commission 2010). LCAs are conducted by LCA practitioners to support decision for making the best possible choice for the environment.

Product systems can include many processes, and in many cases, variations of these processes are possible, which can result in a very large number of possible combinations—or alternative life cycle pathways (PW). Each new PW we regard as an additional solution to the LCA space. In applied LCAs, the potential variations are most often considered in a nonsystematic ad hoc manner, where only a very limited number of variations are considered leading to the risk that more optimal alternatives are overlooked, we call this the “ad hoc LCA approach.” In this article, we present a more systematic approach to the development of the alternatives to investigate in the LCA which we will call the “structural LCA approach”. Here, it becomes possible to create a much larger LCA space compared to the ad hoc LCA approach and, in addition, it opens new options for analyzing and investigating the LCA space with focus on optimization. In the present paper, we apply the “design of experiments” (DOE) methodology based on Montgomery (2005) (Table 1). Since many LCA practitioners use software tools like SimaPro (Pre-sustainability 2012) or GaBi (PE International 2012) for the simulation of the product system, it should not require much more effort to expand the space of alternatives by varying different explanatory variables in the product system model and evaluate the outcome of these changes. The benefits of the structural LCA approach, compared to the ad hoc approach, can be fourfold:

1. Easy expansion of the space of alternatives by developing the structural table.
2. Based on response surface methodology, we can investigate which of the explanatory variables are the most influential for each response variable/impact category and, hence, derive optimal settings for each explanatory variable. This can be done by using statistical software tools (e.g., “R” (R Project 2012) which is freely available). We call this single-objective optimization (SO).
3. If the number of alternatives is sufficiently high, then multiobjective optimization (MO) can be used as a nonsubjective method to find the Pareto optimal alternatives[1] for the system and delimit the use of the often challenged value-based weighting step in the LCA since the LCA practitioners then can avoid the weighting step sometimes used in LCA and then leave the final decision and also implicit valuation of the different option to the decision maker(s). Furthermore, the hypervolume estimation taboo search (HETS) method that was developed for this project enables MO to be used for more than 2–3 objectives which is highly relevant for LCA that may operate with up to 15 different midpoint impact categories (Hauschild et al. 2013).
4. The reporting of the LCA can be more transparent if the explanatory variables are explicitly outlined with a distinction between explanatory variables that have been changed in the study and explanatory variables that have been kept constant (“ceteris paribus” approach).

The structural LCA approach is explained and demonstrated through a well-to-wheel (WTW) study of biodiesel developed within a 3-year LCA research program. Two Danish companies, Emmelev A/S (Emmelev 2012) (biodiesel refinery) and Novozymes A/S (Novozymes 2012) (producer of industrial enzymes), have been partners with focus on the optimization of the environmental performance of biodiesel in a WTW perspective. The WTW biodiesel study has been documented in detail in Herrmann et al. (2012) and reference is given to this source for details on the LCA calculations for this WTW biodiesel study.

2 Methods

First, we outline the structural LCA approach, the SO approach, and the MO approach. Second, we implement these methodologies in the WTW case study of biodiesel.

[1] i.e., nondominated alternatives.

Table 1 Abbreviation and translation between LCA, statistics, and operations research for central concepts in this paper

LCA	Statistics (Montgomery 2005)	Operations research	Abbreviation in this paper
Life cycle assessment			LCA
		Operations research	OR
The structural table	The design		
	Design of experiments		DOE
Functional unit	Normalization		
Pathway, scenario	Run	Solution	PW
LCA space		Space	
Impact categories	Response variables	Objectives	
Product system variables	Explanatory variables		
Option or choice	Level		
Well-to-wheel			WTW
		Single-objective optimization	SO
		Multiobjective optimization	MO

2.1 The structural table

The structural LCA approach is formulated through the structural table as outlined in Table 2. Potentially, we can look at, e.g., 20 different explanatory variables, such as electricity supply and other fundamental technology choices, distance and means of transport, production equipment, additives, products that can be substituted (e.g., petrochemical fuels with biofuels), and production location. Depending on the specific decision support context, these explanatory variables and many other explanatory variables can be of great interest for the LCA practitioners (and decision makers) for potentially changing the environmental impact from a product system. Each explanatory variable can be varied on a discrete or continuous scale. In this section, we only consider discrete options, for example, 20 explanatory variables, each with 4 levels.[2] Without any constraints, this would be a problem of 4^{20} individual alternatives. In the context of LCA, we will consider these alternatives as different PWs through the life cycle, representing (sometimes marginally) different product systems. Many of these PWs might not, at present, be technically possible or economically feasible. On the other hand, if the environmental impact of some of these PW turns out to be considerably low compared to a baseline scenario or business-as-usual scenario, then investments for developing these PW may be interesting to consider. The design of the structural approach is not trivial and is highly dependent on the goal and scope of the LCA. For example, from a decision making point of view, it is relevant to consider how much influence the decision maker can exercise over the different explanatory variables. In an initial "screening" experiment, it can be meaningful to operate with fewer levels than, e.g., four, as the number of PWs rapidly decreases, for example, going from 2^{20} to 4^{20} is an increase of PWs with a factor of ~1.05 million.

2.1.1 Design of the structural table and the application to LCA

An approach for the design of the structural table can be to use an expert panel to determine (Montgomery 2005):

(a) The relevant explanatory variables.
(b) The relevant scale of the levels for each explanatory variable.
(c) The relevant response variables (if not all environmental impact categories).

For practical LCA application, this might be an ongoing process during the LCA project. For illustration purposes, Fig. 1 shows a 2^4 factorial design with electricity, use of straw from field, choice of alcohol,[3] and transport distance of fuel as the four explanatory variables, each with two levels: high (+) and low (−). For alcohol, "–" indicates the choice of bioethanol (BioEt) and "+" indicates the choice of petrochemical methanol (PCMe). Figure 1 is intended as a visual interpretation of how the experiment is structured and it may serve as a way to systematize and keep track of changes of the levels of the different explanatory variables. Two cubes are needed to visualize all the possible settings in a 2^4 factorial design, while only one cube would be needed in a 2^3 factorial design. In Fig. 1, alcohol is visualized as the "fourth" explanatory variable which is then bridging between the two cubes. One

[2] Each of these levels represents a possible setting for the explanatory variables. For example, if the explanatory variable considered is "type of alcohol used," then the two levels can be bioethanol or petrochemical methanol.

[3] Alcohol is needed for producing biodiesel.

Table 2 The structural table

PW	Explanatory variables					Response variables			
	X_1	X_2	…	X_n		Y_1	Y_2	…	Y_m
1	Level 1	Level 1		Level 1	=	Obs. 1	Obs. 1		Obs. 1
2	Level 2	Level 2		…	=	Obs. 2	Obs. 2		…
3	Level 3	…			=	Obs. 3	…		
4	…				=	…			
…					=				
l	Level h	…		…	=	…	…		…

Each pathway has a unique ID number ranging from 1 to *l*. There are *n* explanatory variables. There can be *h* different levels for each explanatory variable. Dependency between the explanatory variables is investigated in the later optimization step. There are *m* different response variables

Obs. Observation (or result)

approach in DOE is to select the starting point, with all explanatory variables at the low level, and then successively vary each variable over its range with the other variables held constant. When using LCA software tools like SimaPro or GaBi, we would have to make a new run (simulation) for each PW with the new setting in our database (or model structure) and read off the new response values. When both the left side of structural table (explanatory variables) and the right side (response variables) are populated with all the data, then several options for analyzing this table, based on SO and MO, becomes possible to support an optimized use of resources and reduced environmental impacts.

In the design in Fig. 1, there are four main effects, one from each explanatory variable. In designs with more than one explanatory variable (2^n, with $n>1$), there is a possibility for dependency between the different explanatory variables; this is called interaction effects. For small designs, say a 2^2 design, it is simple to compute, by hand, both the main effects and the interactions effects. Calculating the effect in a 2^1 design is done by subtracting the response variable value between the high and low levels. However, to compute these effects by hand, it rapidly becomes unrealistic and requires a statistical software tool as the number of explanatory variables. For a general procedure for calculating main effects and interaction effects, we refer to Montgomery (2005).

2.2 Single-objective optimization

By using a statistical software tool, such as "R" (R Project 2012) which is freely available, we can translate the previously discussed structural table into a statistical effect model (Eq. 1). Based on this statistical model, we can investigate and quantify which explanatory variables are the most influential on the specific impact category (response variable). In addition, if the explanatory variables in the LCA are controllable for the decision maker, then the stated model enables us to adjust the explanatory variables to achieve a reduction in the impact category. If the goal of the LCA is to minimize the different environmental impacts, then we can optimize according to these preferences. Equation 1 is the statistical

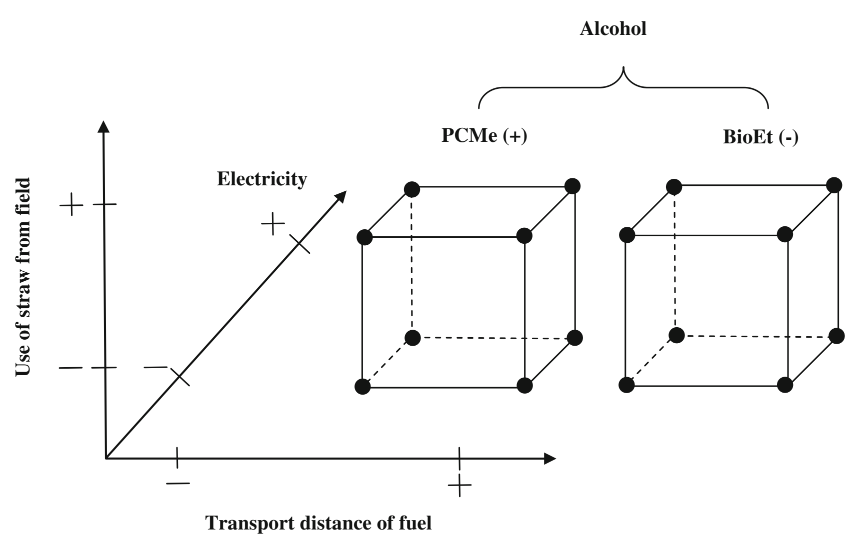

Fig. 1 A full four-factor factorial design with two levels (2^4 design). Each corner in the two cubes (and the ends of the bracket) illustrates the high and low setting for run of the experiment. *PCMe* petrochemical methanol, *BioEt* bioethanol. In the specific LCA context, the different settings of the explanatory variables (such as "Electricity," high or low) correspond to the settings of the LCA product system variables

effect model of a two-factor design, with a levels for explanatory variable τ and b levels for the explanatory variable β:

$$y_{ij} = \mu + \tau_i + \beta_j + (\tau\beta)_{ij} + \varepsilon_{ij} \begin{cases} i = 1, \ 2, \ \ldots, \ a \\ j = 1, \ 2, \ \ldots, \ b \end{cases} \qquad (1)$$

y_{ij} is the observed response when explanatory variable τ is at the ith level (i=1, 2, …, a) and explanatory variable β is at the jth level (j=1, 2, …, b), μ is a parameter common to all changes within the different explanatory variables[4] called the overall mean (or the intercept), $(\tau\beta)_{ij}$ is the interaction effect between τ_i and β_j, and the ε_{ij} is a random error component that incorporates all other sources of variability in the PW, including measurement variability, variability arising from uncontrolled factors, and the general background noise in the processes (such as variability over time, effects of environmental variables, and so forth). The interpretation of this model is that μ is a constant and the effects of changing within the different explanatory variables τ_i, β_j, and the interaction effect $(\tau\beta)_{ij}$ represent deviations from the constant (μ) when the specific changes are applied (Montgomery 2005). When simulating the effects on environmental impacts from an LCA product system through the software tools SimaPro or GaBi, we would not expect any random error effects $(\varepsilon)_{ij}$ to occur. Another way to investigate the potentials for optimization is to calculate the sum of squares (or least square estimates). The sum of squares indicates which of the different explanatory variables that contributes the most to the variation in the structural table. Hence, in the LCA context, the sum of squares also shows which explanatory variables contribute the most to the potential improvement of the environmental impacts from the LCA product system.

2.3 Multiobjective optimization

Using MO in LCA was originally suggested by Azapagic in 1999 (Azapagic 1999; Azapagic and Clift 1999a, b). When dealing with more objectives or goals, there may not be a single solution that is always best; hence, there are trade-offs between the different objectives. For instance, the most environmentally friendly car is rarely the fastest, too. Hence, choosing a best solution depends on preferences for different objectives. This point is illustrated in Fig. 2, where f_1 is speed and f_2 is environmental friendliness. The Pareto front is defined by the solutions that are not dominated by other solutions, i.e., the four white dots in Fig. 2.

Some solutions in Fig. 2 are dominated by the solutions placed on the Pareto front in Fig. 2, meaning that one or more other solutions are better in all objectives. These dominated

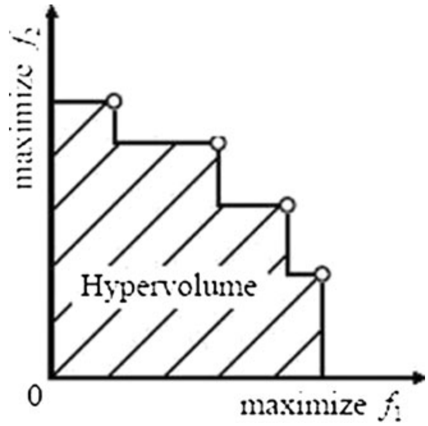

Fig. 2 Illustration of the trade-off between speed (f_1) and environmental friendliness (f_2) in the MO approach. The Pareto front is the border where no solutions are dominated by other solutions, whereas all solutions inside the “Hypervolume” are dominated by solutions on the Pareto front

solutions are naturally undesired, as there is a better alternative. With three objectives, the area in Fig. 1 becomes a volume, and with more objectives, it becomes a hypervolume which is not practically possible to illustrate.

Compared to the SO method, the MO has, at least, one advantage. The SO approach to solve trade-off problems is basically to sum all the objectives with different weights (based on their assumed importance) and then choosing the apparently best solution. The SO method, however, has a serious drawback that makes it an undesirable approach in many optimization problems. The problem with the SO method is that the LCA practitioner or analyst has to provide very good weights, which are practically impossible to determine. The analyst may have an idea of the overall preference, but to put this into exact weights is difficult, and furthermore, the best solution found may not be anything close to the solution that would have been preferred if different solutions had been given to the decision maker.

Traditionally, MO has only been practically possible for two to three objectives. The new method “hypervolume estimation taboo search” (HETS), which is developed for the present project, makes it possible to investigate far more objectives (up to 25 objectives) by using a faster approximation of the hypervolume compared to traditional methods. This makes HETS highly relevant for LCA which sometimes applies up to 15 different impact categories (Hauschild et al. 2013). The developed HETS algorithms have been tested on a range of different datasets with different numbers of objectives and problem sizes. It clearly outperforms traditional methods, such as “Strength Pareto Evolutionary Algorithm” (SPEA-II) (Zitzler et al. 2001), “Nondominated Sorting Genetic Algorithm” (NSGA-II) (Deb et al. 2002), “Simple Evolutionary Multiobjective Optimizer (SEMO) (Laumanns et al. 2002), or “Set Preference Algorithm for Multiobjective Optimization” (SPAM) (Zitzler et al. 2010), in terms of both

[4] Given by varying over the different levels in each of the explanatory variables.

speed and performance which can be measured as the quality of the set of solutions achieved. For a further explanation of the quality of the set of solutions achieved, see Lundberg-Jensen (2011). With fewer objectives (three to eight), the improvement was less significant. Going up to 25 objectives, the improvement was over a factor of 50 in computation time. The HETS method and performance is further documented in Lundberg-Jensen (2011).

3 Well-to-wheel study of biodiesel

The functional unit for the LCA is 1,000 km driving in a passenger diesel car with a blend of 20 % biodiesel (produced from rape seed oil and methanol or BioEt) and 80 % petrochemical diesel (20B). This blend is referred to as "biodiesel" in this paper. The use of the passenger diesel car is based on an Ecoinvent process ("Operation, passenger car, diesel, fleet average 2010/RER U") which reflects a fleet average in Europe in 2010. The study includes tailpipe emissions, biodiesel production, oil production, alcohol production, and rapeseed production—including specific modeling of fertilizer and pesticide emissions. It is assumed in our study that biogenic CO_2 emissions to the atmosphere are balanced out by an equal uptake by growing the crops in the production system (prior to harvest). Hence, all biogenic CO_2 emission is accounted with zero impact, while CO_2 emission originating from PC diesel is accounted as a net contribution to the CO_2 content of the atmosphere. The baseline scenario of rapeseed fatty acid methyl ester is documented in Herrmann et al. (2012). The product system is illustrated in Fig. 3.

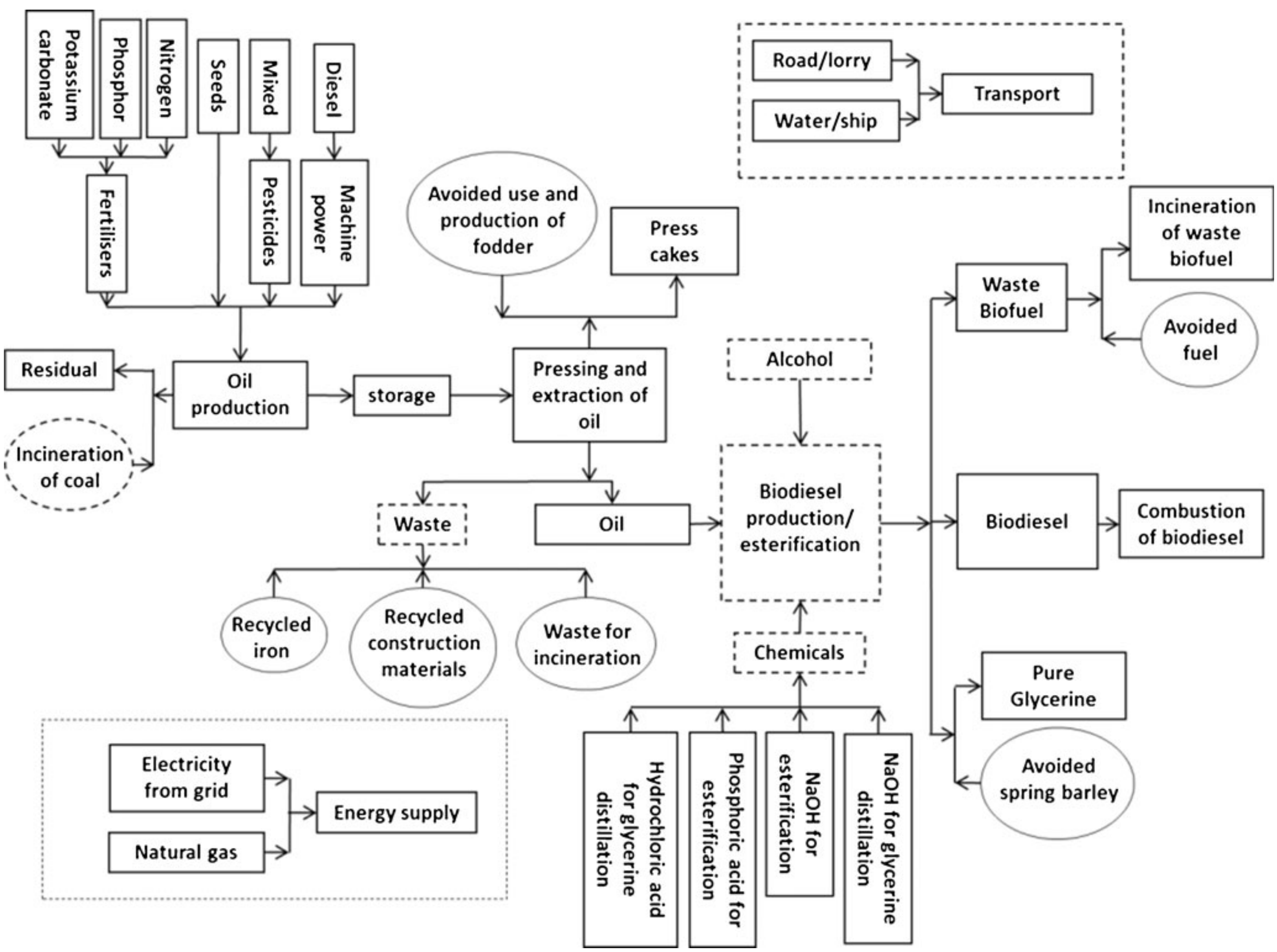

Fig. 3 The analyzed system for the production and combustion of biodiesel for passenger car transport based on different types of diesel (based on Herrmann et al. 2012). Transportation includes road and water transport mainly for the transport of feedstock to the pressing and extraction process. The *dashed lines* illustrate the variables that will or can be changed for creating alternative pathways (PW1–64)—see Table 4

4 Results and discussion

As described in the "Methods" section, the selection of the explanatory variables is or can be an ongoing process. In the present project, we have chosen to demonstrate the structural approach with the six explanatory variables, each with two levels, as presented in Table 3.

The main reasons and assumptions for the level settings are outlined in the following. For the use of fertilizer or manure, we assume that the crop's nitrogen requirement is fixed; hence, we only change the ratio between fertilizer and manure. Increasing the use of fertilizer will result in an increased production of this, which is highly energy demanding. Approximately, there is 3.5 t of straw residual on a land field per year per ha according to the Danish Statistics (2011)) and some of this can be used for co-incineration in a power plant. We assume that using straw in a power plant will substitute coal in the energy ratio of approximately 1:1. Either a conventional or an enzymatic transesterification process can be used. Data for the conventional process is from the operation of Emmelev A/S and data for the enzymatic process is from Novozymes A/S and Sotoft et al. (2010). The production of BioEt and PCMe are based on unit processes from the Ecoinvent database 2.0 (Faist et al. 2007). It is assumed that the production of biodiesel takes place either in Denmark or in Poland which we mainly assume will influence the production of electricity and the transport distance. For further discussion of assumptions and modeling issues, we refer to Herrmann et al. (2012).

Furthermore, we considered a range of other explanatory variables, such as use of pesticides, types of oil feedstock, cleaning technology for tailpipe emission, coproduct substitution options (e.g., glycerol substituting petrochemical glycerol, wheat for feed, or other products; Jørgensen et al. 2012), and fuel types for heat generation. During the decision process (including Novozymes A/S and Emmelev A/S) on the choice of explanatory variables, levels for these explanatory variables, and the choice of response variables, it was decided to use the ones presented in Tables 3 and 4 (the response variables in the right side of the table). The rest of the explanatory variables mentioned previously were thus considered to be fixed or ceteris paribus.

4.1 The structural table

In our case, we used SimaPro as the LCA software for modeling our LCA. We used five different PWs as fundamental PWs which we successively varied to fit each specific PW setting in the structural table (Table 4). Second, we populated the right side of the structural table after simulating the specific PW in SimaPro. After using months for collecting data for the 5 basic PWs, it "only" took a week or less to generate the 64 different PWs presented in Table 4, together with the statistical evaluation of these PWs by the use of "R." PW D0 is petrochemical diesel according to the Ecoinvent database 2.0 (Faist et al. 2007) and PW1 is biodiesel production based on the present conditions according to Herrmann et al. (2012). The full structural table can be found in the Electronic supplementary material.

As the number of explanatory variables of interest or the number of levels for each explanatory variable increases, the number of PWs required being developed increases rapidly; for instance, a 10-factor experiment with 3 levels would require 59,049 PWs. This quickly becomes infeasible from a time and resource viewpoint. In this case, a fractional factorial design can be an alternative to the full factorial design. In a fractional factorial design, only a subset of the PWs is needed (Montgomery 2005). For example, if in Fig. 1 we only had 8 PWs of the 16 possible combinations (illustrated by each corner in the 2 cubes and the ends of the bracket), then this would be a one half fraction or a 2^{4-1} design which then basically saves half the resources to develop PWs. The trade-off in fractional designs, which becomes more expressed in larger designs, is that some of the lower-order interaction effects will be confounded with higher-order effects (such as main effects), and if some of these interaction effects are

Table 3 The six explanatory variables used for the illustration of optimization of biodiesel production and use

Levels	Fertilizer mix (fertilizer/manure)	Removal of straw for incineration in t/(ha year)	Transesterification process	Alcohol	Electricity	Transport of biodiesel
Low (−)	0.3/0.7	0	Conv.	BioEt	DK	150 km by lorry
High (+)	0.5/0.5	1	Enz.	PCMe	PL	200 km by lorry and 750 km by ship
Present	0.34/0.66	0.52	Conv.	PCMe	DK	+/−

Conv. conventional, *Enz.* enzymatic, *DK* Denmark, *PL* Poland

Table 4 The structural table based on the full factorial 2^6 design (PW1–64)

PW	Explanatory variables							Response variables				
	Fert. mix	Use of straw	Transesterification process	Alc.	Elec.	Tran.		Climate change	Land use	Respiratory inorganics	Human toxicity (carc.)	Aquatic eutrophication N
D0	NA	NA	NA	NA	NA	NA	=	214.0	0.2	0.0870	1.08E−06	0.06
0	Pre.	Pre.	Pre.	Pre.	Pre.	Pre.	=	57.0	89.8	0.0473	1.50E−06	0.57
1	−	−	Enz.	BioEt	DK	−	=	81.4	101.0	0.0707	1.57E−06	0.55
2	−	−	Enz.	BioEt	DK	+	=	93.2	101.0	0.0798	2.16E−06	0.56
3	−	−	Enz.	BioEt	PL	−	=	82.8	101.0	0.0738	1.64E−06	0.55
4	−	−	Enz.	BioEt	PL	+	=	94.7	101.0	0.0828	2.24E−06	0.56
5	−	−	Enz.	PCMe	DK	−	=	93.0	83.7	0.0483	1.19E−06	0.56
6	−	−	Enz.	PCMe	DK	+	=	105.0	83.7	0.0571	1.85E−06	0.57
7	−	−	Enz.	PCMe	PL	−	=	94.8	83.7	0.0528	1.31E−06	0.56
8	−	−	Enz.	PCMe	PL	+	=	106.0	83.7	0.0617	1.97E−06	0.57
9	−	−	Conv.	BioEt	DK	−	=	78.7	103.0	0.0718	1.86E−06	0.56
…	…	…	…	…	…	…	=	…	…	…	…	…
64	+	+	Conv.	PCMe	PL	+	=	43.6	83.6	0.0638	2.61E−06	0.59

The full structural table is to be found in the Electronic supplementary material. The specific settings of the different levels are given in Table 3. For example, "−" for the explanatory variable "Fert. mix" means a ratio of 0.3/0.7 fertilizer/manure mix, as can be seen in Table 3

Fert. fertilizer, *Alc.* alcohol, *Elec.* electricity, *Tran.* transport of biodiesel, *Pre.* present, *NA* not applicable

significant, then this can potentially blur the interpretation of the resulting statistical model. As the numbers of explanatory variables increases, it becomes more complicated to make elegant fractional designs, where as few as possible lower-order interaction effects are confounded with higher-order effects. Some suggestions for these designs can be found in reference books. For example, in Montgomery (2005), a $2^{15\text{-}11}$ fractional design can be found which is a 1/2,048 fraction of the full design.

4.2 Single-objective optimization

In the following, two objectives are analyzed for optimization potentials, namely, climate change potentials (Table 5) and respiratory inorganics (Table 6). The raw output files from R, which was used to analyze the data, are found in the Electronic supplementary material. We observed only insignificant interaction effects, and hence, these were taken out of the final model according to the principle of parsimony (Crawley 2005).

Table 5 Optimization potentials of climate change potential based on effect estimates and sum of squares

	Effect estimate [kg CO_2 eq.]	Sum of squares	Percent contribution
Intercept (μ)	79.54		
Fert. (+)	13.20	2,788	3.0
Straw (+)	−73.55	86,554	92.3
Trans. (enz)	2.28	83	0.1
Alc. (PCMe)	11.13	1,982	2.1
Electricity (PL)	1.66	44	0.0
Transp. (+)	12.06	2,328	2.5

Tables 5 and 6 are divided into four columns: the explanatory variables with an indication of the contribution direction, i.e., high (+) or low (−); the effect estimates which are the coefficients in Eq. 1; the sum of squares which can be interpreted as the variation contribution based on the structural table; and the percent contribution to the variation based on the sum of squares, that is, the sum of square for each explanatory variable divided by the total sum of squares. The first row in the table is the intercept or the mean value (μ) in Eq. 1. The intercept is (in this model) a somewhat arbitrary size which is determined by the model we have constructed. In Table 5, we see that changing the ratio of fertilizer versus manure from the low ratio to the high ratio (0.5/0.5) will, in response (on average), increase the climate change potential with 13.20 kg CO_2 eq. If we change the removal of straw, from the field and use it for incineration in a power plant which in return will substitute coal, from 0 to 1 t/(ha year), then we will (on average) decrease the climate change potential with 73.6 kg CO_2 eq. If we look at the columns with sum of squares and the percent contribution for sources of variation, then we can see that the use of straw is by far the main contributor to the variation of the climate change potential. In a decision support context, this indicates where the main

Table 6 Optimization potentials of respiratory inorganics based on effect estimates and sum of squares

	Effect estimate [kg 2.5PM eq.]	Sum of squares	Percent contribution
Intercept (μ)	0.0711844		
Fert. (+)	0.0070750	0.0008009	7.0
Straw (+)	−0.0048688	0.0003793	3.3
Trans. (enz)	−0.0002000	0.0000006	0.0
Alc. (PCMe)	−0.0230313	0.0084870	74.6
Electricity (PL)	0.0043188	0.0002984	2.6
Transp. (+)	0.0093750	0.0014062	12.4

potential for optimized production and use of biodiesel is to be found. As indicated in the "Methods" section, if the decision maker cannot exercise power over a given explanatory variable, then this information might be of less interest. In contrast to "the use of straw from the field" variable, we see that the transesterification process or use of electricity in a life cycle perspective, based on our data, contributes with little improvement (or change) to the overall climate change impact.

Regarding the transesterification process, it is important to notice that the conventional process is a mature technology that has been developed over the last decades, while the enzymatic process is a new technology. If the enzymatic processes are developed further, we would expect that there will be a higher potential for improving this technology compared to the already mature and conventional transesterification process. We have made no attempt to predict (or forecast) these potentials. The enzymatic process is based on immobilized enzyme catalysts. Other enzyme processes, including those based on liquid enzyme formulations, could lead to somewhat different results.

Table 6 presents the optimization potentials for respiratory inorganics. We see that fertilizer and use of straw contribute to the impact potentials in the same "direction" as for the climate change potentials, i.e., increasing the use of fertilizer and straw will increase and decrease, respectively, the respiratory inorganics potentials. On the other hand, we see that, where the type of alcohol had relatively little influence on the climate change potential, then it is the main contributor to the respiratory inorganics impact potentials. In addition, we see that the type of alcohol contributes in the opposite direction to the impact potential than for the climate change potential. This gives some trade-off consideration when deciding on optimized production and use of biodiesel, based on SO. However, one of the main reasons that BioEt relatively to PCMe has such a high effect on the respiratory inorganics impact category is that, in the production of BioEt, workers in the sugar cane fields are highly exposed to particles contributing to this impact category. Hence, there seems to be a rather large potential to minimize the respiratory inorganics impact from BioEt (by improved production practices or different shielding technologies) which can reduce the trade-off between the respiratory inorganics impact category and the climate change impact category. For further analysis of origin of sources to the different impact categories, we refer to Herrmann et al. (2012).

When going from the ad hoc LCA approach to the structural LCA approach, SO becomes possible to use for analyzing data. MO is another optimization method that becomes possible to use when applying the structural LCA approach. In addition, MO can solve some of the previously discussed problems that we see with SO of finding the best possible combination, i.e., minimizing the trade-offs when selecting one or more PWs for further investigation.

4.3 Multiobjective optimization

The Pareto optimal front is given in Table 7 by the five PWs which are not dominated by other solutions as indicated in the column "Dominated" by a "No" (while all dominated solutions are indicated by a "Yes"). This number (five) indicates that there is no intuitive solution that dominates all other solutions. At the same time, the number of optimal solutions is still a fairly small part of the total solution space. This means that the MO approach is useful not only to find which solutions best represent the Pareto front but also to actually find the Pareto optimal solutions (unlike when close to all solutions turn out to be optimal in some way). The full Table 7 can be found in the Electronic supplementary material.

With the ad hoc LCA approach, these specific five PWs (D0, 17, 21, 25, and 29) would not immediately have been identified as optimal solutions. From a decision making point of view, we can probably also exclude PW25 since no conventional transesterification that can handle ethanol is likely to be developed in the nearest feature. This can further reduce the Pareto front with one PW. Also, considering the supply safety (which is an often mentioned problem for petrochemical fuels), then D0 (petrochemical diesel) can be taken out, too.

4.4 The ad hoc LCA approach versus the structural LCA approach

It is important to notice that the structural LCA approach is not a substitute for the ad hoc LCA approach but an additional analysis that can be performed given that the data has already been collected (for the ad hoc LCA approach). In most LCA studies, however, there is normally the option of improving the data quality (for the ad hoc approach). Given that the LCA practitioner has a fixed amount of resources,[5] then it becomes a matter of prioritizing between additional development of the

[5] e.g., 2 months to perform an LCA study.

Table 7 The MO approach gives the Pareto optimal front (PW: D0, 17, 21, 25, and 29)

PW	Explanatory variables						Response variables					
	Fert. mix	Use of straw	Transesterification process	Alc.	Elec.	Tran.	Climate change	Land use	Resp.	HTox.	Aq. N	Dominated
D0	NA	NA	NA	NA	NA	NA	214.0	0.2	0.0870	1.08E−06	0.06	No
…	…	…	…	…	…	…	…	…	…	…	…	…
17	−	+	Enz.	BioEt	DK	−	10.0	98.7	0.0660	1.41E−06	0.55	No
21	−	+	Enz.	PCMe	PL	−	18.5	81.7	0.0434	1.03E−06	0.56	No
25	−	+	Conv.	BioEt	DK	−	6.3	101.0	0.0670	1.70E−06	0.55	No
29	−	+	Conv.	PCMe	PL	−	15.9	83.4	0.0434	1.30E−06	0.57	No
…	…	…	…	…	…	…	…	…	…	…	…	…
61	+	+	Conv.	PCMe	DK	−	29.5	83.6	0.0504	1.88E−06	0.58	Yes
62	+	+	Conv.	PCMe	DK	+	42.1	83.6	0.0600	2.55E−06	0.59	Yes
63	+	+	Conv.	PCMe	PL	−	31.0	83.6	0.0541	1.98E−06	0.58	Yes
64	+	+	Conv.	PCMe	PL	+	43.6	83.6	0.0638	2.61E−06	0.59	Yes

Resp. respiratory inorganics, *Htox* human toxicity (carc.), *Aq. N* aquatic eutrophication N

ad hoc LCA or, at the end of a project period, applying the structural LCA approach with the benefits that can follow from that. This choice will depend on the goal and scope of the LCA. For example, if the LCA is to be used for internal decision support in a company which only has power to change a single explanatory variable, then it would be more or less pointless to apply this new structural LCA approach, since the benefits from the structural LCA approach mainly relates to a situation where the decision maker can influence more explanatory variables. In the case where the decision maker can exercise power over more explanatory variables, it might become beneficial to apply the structural LCA approach to identify the explanatory variables that have the highest potentials for reducing the environmental impact in an LCA perspective and to quantify the potentials. In other words, the structural LCA approach can be used to illuminate where the "low-hanging fruits" might be. This can especially be of interest if the LCA is communicated to a broader range of stakeholders, including decision makers at the societal level.

If the LCA is viewed as an ongoing process, then the potentials for the different explanatory variables change over time as stakeholders/society realize the improvement potentials. For example, if the use of straw is changed from the present situation to a situation where it reaches its limit given by biophysical carbon sequestration constraints and market-related constraints, such as competing use of the straw and (missing) economic incentives for use of the straw for power generation, then the magnitude of the potentials for the other explanatory variables will increase.

Potentially, some LCA experts and practitioners, based on the ad hoc LCA approach, could have deduced some of the information presented in Tables 5, 6, and 7 by the expert knowledge that they already have. However, in general, it had not been possible with the ad hoc approach to quantify the magnitude of the potentials for each explanatory/response variable and find the Pareto front, as done with the structural LCA approach.

The structural LCA approach (based on optimization methodology and DOE) thus has a different purpose than a typical use of scenario analysis or Monte Carlo analysis in LCA. While the structural LCA approach is used for identifying actual options for improvement options throughout the life cycle, Monte Carlo analysis is typically used in LCA to determine uncertainty propagation and quantify overall uncertainties. Scenario analysis is often used for analyzing large-sized projects with structural and policy changes in mind—also considering longer time horizons, maybe 20–30 years, and including "the consequence of the consequence of the …," i.e., not with the purpose of optimizing but as a "what if analysis" in an ad hoc manner.

4.5 Application to published LCA studies

The structural LCA approach has been outlined and demonstrated on an LCA biodiesel case based on Herrmann et al. (2012). In the following, three published LCA studies are identified where it would have been possible to apply the structural LCA approach, of course depending on the goal and scope of the studies and the resources available for the LCA practitioner. Harding et al. (2008)) make a life cycle comparison between inorganic and biological catalysis for the production of biodiesel. Five different PWs are assessed in this paper and these PWs are evaluated based on ten different impact categories. With a few permutations of the five different PWs, it would have been possible to increase the LCA space (significantly) and screen the LCA space for

optimal solutions based on the structural LCA approach. Similarly, Restianti and Gheewala (2012) present an LCA of gasoline in Indonesia based on six impact categories. Also, in this paper, it would have been possible to apply the structural LCA approach both with regard to SO and MO. Ziegler et al. (2012) evaluate the carbon footprint of Norwegian seafood products on the global seafood market. In this paper, only the carbon footprint is applied as assessment criterion, while there are approximately eight different explanatory variables identified for the production and distribution system of Norwegian seafood products. Here, the structural LCA approach used for the purpose of single optimization would have been possible to apply, too.

5 Conclusions

The use of the structural LCA approach for optimization purposes was demonstrated based on different optimization approaches, such as SO and MO. In addition, the structural LCA approach can lead to more transparent LCAs since the explanatory variables[6] which are used to model the LCAs are explicitly presented through the structural LCA approach. At the same time, all other explanatory variables, both known and unknown, are kept constant or ceteris paribus which in turn gives the reader a clear insight into which are included as changing explanatory variables and which explanatory variables (all others) are kept constant.

Given that there is a fixed amount of resources available for the LCA practitioner, it becomes a prioritizing problem whether to apply the structural LCA approach or not. If the decision maker can only change a single explanatory variable, it might not be beneficial to apply the structural LCA approach. However, if the decision maker (such as decision makers at the societal level) has the power to change more explanatory variables, then the structural LCA approach seems beneficial for quantifying and comparing the potentials for environmental improvement between the different explanatory variables in an LCA system.

In the present analysis of biodiesel in a WTW perspective, and based on SO, we found that the most important explanatory variable for climate change potential, compared to the other explanatory variables, is the “use of residual straws from fields” which can be used for co-incineration in power plants and hereby substituting coal. For the respiratory inorganics impact category, the use of alcohol contributes the most to the variation and, hence, improvement potential for this impact category, compared to the other explanatory variables used for optimization potential identification. Based on MO, we found the Pareto front consisting of five PWs (D0, 17, 21, 25, and 29) which are not dominated solutions out of the 66 different PWs.

[6] At least the potential most important explanatory variables.

6 Outlook

The suggested structural LCA approach seems to be a promising approach for searching or screening product systems for environmental optimization potentials. In the presented case, the design has been a rather simple full factorial design. The application to more complicated problems or designs, such as fractional designs, nested designs (i.e., where not all levels in an explanatory variable can substitute one another), split plot designs, and/or unbalanced data is an obvious possibility that should be investigated further in the context of LCA.

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